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Wigner–Weyl correspondence in quantum mechanics for continuous and discrete systems—a Dirac-inspired view

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Abstract

Drawing inspiration from Dirac's work on functions of non-commuting observables, we develop an approach to phase-space descriptions of operators and the Wigner–Weyl correspondence in quantum mechanics, complementary to standard formulations. This involves a two-step process: introducing phase-space descriptions based on placing position dependences to the left of momentum dependences (or the other way around); then carrying out a natural transformation to eliminate a kernel which appears in the expression for the trace of the product of two operators. The method works uniformly for both continuous Cartesian degrees of freedom and for systems with finite-dimensional state spaces. It is interesting that the kernel encountered is naturally expressible in terms of geometric phases, and its removal involves extracting its square root in a suitable manner.

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1. Introduction

The development of classical phase-space methods to describe quantum systems whose kinematics is governed by Cartesian variables has its origin in two independent ideas. The first, due to Weyl [1], is the setting up of a rule that maps each (real) classical dynamical variable into a corresponding (Hermitian) operator for the quantum system in a linear manner. The second, due to Wigner [2], is the definition of a (real) phase-space distribution function representing each (pure or mixed) quantum state in a complete manner. Later work [3] clarified that these two rules or definitions are exactly inverses of one another, as a result of which quantum mechanical expectation values can be written in a classical-looking form as phase-space integrals.

As a function on the classical phase space, the Wigner distribution is real but not necessarily pointwise non-negative. Therefore, it cannot be interpreted as a probability distribution. It does, however, lead to the correct marginal position and momentum probability distributions given by quantum mechanics.

Inspired by the continuous case, there has been considerable interest in extending the Wigner distribution method to the case of finite-dimensional quantum systems [4–14]. Among the early efforts are the works of Hannay and Berry [4], Feynman [5] and Wootters [6]. In the Hannay–Berry approach, one arrives at the finite-dimensional case by starting from the continuous case and carrying out a process of quotienting with respect to a commutative group of discrete phase-space translations. In Feynman's work the two-dimensional case was treated using the properties of spin in quantum mechanics. Wootters dealt separately with the cases where the dimension of the state space is a power of 2, and where it is odd. In the latter, the odd prime dimension is handled first, and then the general odd dimension by forming a Cartesian product of the prime cases. The approach of Jagannathan [7] is based on the Weyl-ordered unitary operators for translations on a phase-space lattice, leading to the discrete Wigner distribution through the associated characteristic function. The more recent independent work of Luis and Peřina [13] uses a similar approach, and presents a thorough analysis of the problem.

In an interesting paper developing the analogies between classical and quantum mechanics, Dirac [15] discussed the general problem of expressing a quantum dynamical variable, an operator, as a function of the basic complete and irreducible set of operators of the quantum system. The latter forms a non-commutative set, leading to the concept of ordering rules in forming their functions. In this context, Dirac used a description of an operator by a collection of mixed matrix elements, the rows and columns labelled by two different orthonormal bases for the Hilbert space of the system.

The purpose of the present paper is to show that one can arrive at the Weyl–Wigner formalism and results in the continuous case starting from Dirac's ideas and following an elementary series of steps. This illuminates the use of phase-space language for quantum mechanics from an alternative perspective. It is known that if one asks for a phase-space description of a quantum state obeying a small number of very reasonable conditions, then the Wigner distribution is the unique answer. In another direction, in important work by several authors [16] the Weyl–Wigner formalism has been shown to be one of several different possibilities all based on the use of phase-space methods. In the light of this, an alternative line of argument leading to the same answer may be of interest. We then go on to show that the same approach based on Dirac's method works in the finite-dimensional case as well. All desirable features including traciality and recovery of the marginals can be incorporated. The method works uniformly for all dimensions N, as was the case in the Hannay–Berry and Jagannathan treatments. In the qubit case $N = 2$, the earlier results of Feynman and of Wootters are recovered.

Phase-space distributions have also played a significant role in optics, particularly in unifying radiometry and radiative transfer with the theory of partial coherence. These activities were triggered by the pioneering work of Walther on radiometry and that of Wolf on radiative transfer. Walther introduced two definitions for the radiance function. The first definition [17] is analogous to the Wigner distribution and, indeed, the reader's attention was drawn by the author to this fact. Walther's second definition [18], which has since been used in hundreds of radiometry papers may be seen, in retrospect, to be analogous to the Dirac-inspired view of phase-space distributions to be developed here. Interestingly, this remark applies equally well to Wolf's expression for the specific intensity [19], having been inspired by the second definition of Walther.

The value of developing the alternative Dirac-inspired approach in the known and familiar cases is that it may suggest modifications to other quantum mechanical situations of a non-Cartesian type. We have in mind for instance quantum mechanics on Lie groups [20], non-commutative geometric quantum schemes, q-quantum kinematics, etc. In a series of insightful papers [21], the close connection between Wigner distributions and mutually unbiased bases [22] has been brought out. Such bases in turn are known to be related to affine planes in finite geometries, mutually orthogonal arrays, complex polytopes and finite designs [23]. The approach developed here may provide a new perspective to some of these questions and interrelations.

A brief summary of the present work is as follows. After a quick review of the Dirac-inspired phase-space description of operators in quantum mechanics in section 2, in section 3 we show how the trace of the product of two operators can be expressed as a phase-space integral in terms of their phase-space representatives in such a way that the inherent symmetry of the trace operation is manifest. We show that this can be done at the expense of introducing a kernel. We investigate the properties of this kernel in detail and show how by defining a square root of the kernel in a special way one is naturally led to the definition of Wigner distribution and associated phase-point operators. In section 4, we set up the kinematics of an N-level quantum system and examine again the trace of the product of two operators. Expressing this in a manifestly symmetric phase space form brings in an $N^2 \times N^2$ matrix kernel whose properties are studied in section 5. In section 6 we show how, by taking the 'square root' of this matrix kernel in a manner ensuring the recovery of the two marginal distributions and quite similar to the continuous case, one obtains Wigner distributions for any system with a finite-dimensional Hilbert space. The residual sign ambiguities in the result are pointed out. Section 7 treats the $N = 2$ qubit case as an illustration. Section 8 contains the concluding remarks including a comparison with the Hannay–Berry approach.

2. Dirac type phase-space descriptions of operators

We consider a one-dimensional quantum system whose basic operators are a Hermitian Cartesian pair $\widehat{q}, \widehat{p}$ obeying the Heisenberg commutation relation

$$[\widehat{q}, \widehat{p}] = \mathrm{i}\hbar. \tag{1}$$

For corresponding classical phase-space variables as well as particular classical values or quantum eigenvalues, we use $q, q', q'', \ldots, p, p', p'', \ldots$. The continuum-normalized eigenstates $|q\rangle, |p\rangle$ of $\widehat{q}$ and $\widehat{p}$ obey as usual:

$$\langle q|q'\rangle = \delta(q - q'), \qquad \langle p|p'\rangle = \delta(p - p'), \qquad \langle q|p\rangle = (2\pi\hbar)^{-1/2} \exp(\mathrm{i}qp/\hbar). \tag{2}$$

From the completeness relations

$$\int_{-\infty}^{+\infty} \mathrm{d}q |q\rangle\langle q| = \int_{-\infty}^{+\infty} \mathrm{d}p |p\rangle\langle p| = \mathbb{I}, \tag{3}$$

we obtain immediately the two operator statements

$$\delta(\widehat{q} - q) = |q\rangle\langle q|, \qquad \delta(\widehat{p} - p) = |p\rangle\langle p|. \tag{4}$$

Consider now a quantum-mechanical operator $\widehat{A}$. It can certainly be completely described by its position-space matrix elements $\langle q'|\widehat{A}|q\rangle$ which constitute in general a non-local kernel. (In case $\widehat{A}$ is unitary, $\langle q'|\widehat{A}|q\rangle$ is the overlap between eigenstates of the 'old' position operator $\widehat{q}$ and a 'new' one: $\widehat{q}' = \widehat{A}\widehat{q}\widehat{A}^{-1}$, and then the kernel of $\widehat{A}$ would be the exponential of (i times) the analogue of the classical generating function of a canonical transformation of the type '$q - Q$' [24].) The kernel corresponding to $\widehat{A}^{\dagger}$ is

$$\langle q'|\widehat{A}^{\dagger}|q\rangle = \langle q|\widehat{A}|q'\rangle^{*}. \tag{5}$$

To move towards a description of $\widehat{A}$ at a classical phase-space level it is natural to consider, in the spirit of Dirac [24], the mixed matrix element $\langle q|\widehat{A}|p\rangle$ which, regarded as a function of the phase-space variables q and p, certainly also describes $\widehat{A}$ completely. For later convenience, we include a non-vanishing plane wave factor and define the 'left' phase-space representative of $\widehat{A}$ as the function

$$\begin{aligned} A_l(q,p) &= \langle q|\widehat{A}|p\rangle\langle p|q\rangle = \mathrm{Tr}\{\widehat{A}|p\rangle\langle p|q\rangle\langle q|\} \\ &= \mathrm{Tr}\{\widehat{A}\delta(\widehat{p}-p)\delta(\widehat{q}-q)\} \\ &= (2\pi\hbar)^{-1/2}\langle q|\widehat{A}|p\rangle\exp(-\mathrm{i}qp/\hbar). \end{aligned} \tag{6}$$

Here $\langle p|q\rangle$ is the kernel of the unitary operator corresponding to the Fourier transformation, which interchanges $\widehat{q}$ and $\widehat{p}$. It is interesting to note that in Dirac's treatment [24] $A_l(q,p)$ is regarded essentially as the *ratio* $\langle q|\widehat{A}|p\rangle/\langle q|p\rangle$, which determines the form of $\widehat{A}$ as a function of $\widehat{q}$ and $\widehat{p}$ in standard ordered form, i.e. $\widehat{q}$ to the left of $\widehat{p}$.

Even if $\widehat{A}$ is Hermitian, $A_l(q,p)$ is in general complex. However, we do have, as is particularly obvious from the second line in equation (6), the marginals and trace properties

$$\begin{aligned} &\int \mathrm{d}p\, A_l(q,p) = \langle q|\widehat{A}|q\rangle, \qquad \int \mathrm{d}q\, A_l(q,p) = \langle p|\widehat{A}|p\rangle, \\ &\mathrm{Tr}\{\widehat{A}\} = \int\!\!\int \mathrm{d}q\,\mathrm{d}p\, A_l(q,p). \end{aligned} \tag{7}$$

As an alternative to the above, the 'right' phase-space representative of $\widehat{A}$ is given by

$$\begin{aligned} A_r(q,p) &= \langle p|\widehat{A}|q\rangle\langle q|p\rangle = \mathrm{Tr}\{\widehat{A}|q\rangle\langle q|p\rangle\langle p|\} \\ &= \mathrm{Tr}\{\widehat{A}\delta(\widehat{q}-q)\delta(\widehat{p}-p)\} \\ &= (2\pi\hbar)^{-1/2}\langle p|\widehat{A}|q\rangle\exp(\mathrm{i}qp/\hbar). \end{aligned} \tag{8}$$

This is related to expressing $\widehat{A}$ in anti-standard form, $\widehat{p}$ to the left of $\widehat{q}$, and we have again

$$\begin{aligned} &\int \mathrm{d}p\, A_r(q,p) = \langle q|\widehat{A}|q\rangle, \int \mathrm{d}q\, A_r(q,p) = \langle p|\widehat{A}|p\rangle, \\ &\mathrm{Tr}\{\widehat{A}\} = \int\!\!\int \mathrm{d}q\,\mathrm{d}p A_r(q,p). \end{aligned} \tag{9}$$

Thus, we have two phase-space descriptions of the operator $\widehat{A}$ on the same footing, with the roles of coordinate and momentum interchanged to go from one to the other. As noted above, even in the Hermitian case in general both $A_l(q,p)$ and $A_r(q,p)$ are complex. More generally, under Hermitian conjugation we have

$$\widehat{B} =: \widehat{A}^{\dagger} \quad \Rightarrow \quad B_r(q,p) = A_l(q,p)^{*}, \tag{10}$$

so in the Hermitian case we have

$$\widehat{A}^{\dagger} = \widehat{A} \quad \Rightarrow \quad A_r(q,p) = A_l(q,p)^{*}. \tag{11}$$

We can now ask if we can pass in a natural way to a third phase-space description of $\widehat{A}$ standing exactly 'midway' between $A_l(q,p)$ and $A_r(q,p)$, thus treating $\widehat{q}$ and $\widehat{p}$ symmetrically. This is achieved in the next section.

3. Operator product traces and passage to the Weyl–Wigner description

Consider two generally non-commuting operators $\widehat{A}$ and $\widehat{B}$. The trace of their product is symmetric under their interchange and can be expressed in two ways using classical phase space[7]:

$$\begin{aligned}\mathrm{Tr}\{\widehat{A}\widehat{B}\} &= \int\int \mathrm{d}q\,\mathrm{d}p\langle q|\widehat{A}|p\rangle\langle p|\widehat{B}|q\rangle \\ &= 2\pi\hbar\int\int \mathrm{d}q\,\mathrm{d}p\,A_l(q,p)B_r(q,p) \\ &= 2\pi\hbar\int\int \mathrm{d}q\,\mathrm{d}pA_r(q,p)B_l(q,p).\end{aligned} \tag{12}$$

The last line follows from the previous one by symmetry under interchange of $\widehat{A}$ and $\widehat{B}$. However, in each of these two phase-space integrals the manifest symmetry in $\widehat{A}$ and $\widehat{B}$ is lacking. One can ask if such symmetry can be restored while continuing to work with phase-space quantities. Towards this end, we begin by first expressing $(\widehat{A}\widehat{B})_l(q,p)$ entirely in terms of $A_l(q',p')$ and $B_l(q'',p'')$:

$$\begin{aligned}(\widehat{A}\widehat{B})_l(q,p) &= \langle q|\widehat{A}\widehat{B}|p\rangle\langle p|q\rangle = \int\int \mathrm{d}q'\,\mathrm{d}p'\langle q|\widehat{A}|p'\rangle\langle p'|q'\rangle\langle q'|\widehat{B}|p\rangle\langle p|q\rangle \\ &= \int\int \mathrm{d}q'\,\mathrm{d}p'A_l(q,p')K_l(q,p';q',p)B_l(q',p), \\ K_l(q,p';q',p) &= (2\pi\hbar)^2\langle q|p'\rangle\langle p'|q'\rangle\langle q'|p\rangle\langle p|q\rangle = \exp\{\mathrm{i}(q-q')(p'-p)/\hbar\},\end{aligned} \tag{13}$$

the first line in the definition of K_l following from: $\langle q|\widehat{A}|p'\rangle = A_l(q,p')/\langle p'|q\rangle$ and from: $1/\langle p'|q\rangle = 2\pi\hbar\langle q|p'\rangle$. The non-local convolution involved in expressing $(\widehat{A}\widehat{B})_l$ in terms of A_l and B_l is an indication already of the general situation since we are dealing with mixed matrix elements; it is a forerunner of the Moyal or 'star' product when the transition to the Weyl–Wigner description of operators is completed. We may also note that, aside from the continuum normalization of the $\widehat{q}$ and $\widehat{p}$ eigenvectors, the kernel K_l is a four-vertex Bargmann invariant [25]. Hence its phase, which is the area of the phase-space rectangle with vertices (q,p), (q,p'), (q',p) and (q',p'), is a geometric phase[8]. Now combining equation (13) with equation (7) and relabelling some variables for convenience, we get $\mathrm{Tr}\{\widehat{A}\widehat{B}\}$ entirely in terms of left representatives:

$$\mathrm{Tr}\{\widehat{A}\widehat{B}\} = \int\int\int\int \mathrm{d}q\,\mathrm{d}p\,\mathrm{d}q'\,\mathrm{d}p'A_l(q,p)K_l(q,p;q',p')B_l(q',p'). \tag{14}$$

The kernel $K_l\,(q,p;q',p')$ is explicitly symmetric under: $(q,p) \longleftrightarrow (q',p')$, so we have a classical phase-space expression for $\mathrm{Tr}\{\widehat{A}\widehat{B}\}$ manifestly symmetric in $\widehat{A}$ and $\widehat{B}$, but at the cost of a kernel. In addition to symmetry, this kernel possesses two important properties: it is invariant under phase-space translations as it depends only on the differences $q-q'$, $p-p'$, and it satisfies the 'marginals' equations

$$\int \mathrm{d}p'K_l(q,p;q',p') = 2\pi\hbar\delta(q-q'), \qquad \int \mathrm{d}q'K_l(q,p;q',p') = 2\pi\hbar\delta(p-p'). \tag{15}$$

[7] Thus, as is well known, from the point of view of trace calculations the standard and anti-standard orderings are dual to one another.

[8] The connection between Bargmann invariants and geometric phases is explored in [26].

The most natural question is to ask if this kernel can in some sense be 'transformed away' while maintaining manifest symmetry in $\widehat{A}$ and $\widehat{B}$. This can be done if we can express it as the 'square' or the convolution of some more elementary kernel, say in the form

$$K_l(q,p;q',p') = \int\!\!\int \mathrm{d}q''\,\mathrm{d}p''\,\xi(q'',p'';q,p)\xi(q'',p'';q',p'). \tag{16}$$

From the known properties of $K_l(q,p;q',p')$ we can demand that $\xi(q,p;q',p')$ too be a symmetric function of its (pairs of) arguments, be invariant under phase-space translations and so depend only on the differences $q-q'$, $p-p'$ and possess the 'marginals' property

$$\begin{aligned}\int \mathrm{d}p'\,\xi(q,p;q',p') &= \sqrt{2\pi\hbar}\,\delta(q-q'),\\ \int \mathrm{d}q'\,\xi(q,p;q',p') &= \sqrt{2\pi\hbar}\,\delta(p-p').\end{aligned} \tag{17}$$

Easy calculation shows that the expression

$$\xi(q,p;q',p') = \sqrt{\frac{2}{\pi\hbar}}\exp\{2\mathrm{i}(q-q')(p-p')/\hbar\} \tag{18}$$

obeys all the conditions imposed above[9]. If we use this in equation (14) and associate one factor of ξ each with A_l and B_l we arrive at the simpler expression

$$\mathrm{Tr}\{\widehat{A}\widehat{B}\} = \frac{1}{2\pi\hbar}\int\!\!\int \mathrm{d}q\,\mathrm{d}p\,A(q,p)B(q,p), \tag{19}$$

where $A(q,p)$ arises from $A_l(q,p)$ via

$$A(q,p) = \sqrt{2\pi\hbar}\int\!\!\int \mathrm{d}q'\,\mathrm{d}p'\,\xi(q,p;q',p')A_l(q',p') \tag{20}$$

and similarly for $B(q,p)$.[10] We have thus achieved, by a two-step procedure, our objective of expressing $\mathrm{Tr}\{\widehat{A}\widehat{B}\}$ as a manifestly symmetric classical phase-space integral, with one phase-space function each representing $\widehat{A}$ and $\widehat{B}$ and with no additional kernel. One can now see that in the case $\widehat{A}^\dagger = \widehat{A}$, $\widehat{B}^\dagger = \widehat{B}$, since $\mathrm{Tr}\{\widehat{A}\widehat{B}\}$ is real and $\widehat{A}$ and $\widehat{B}$ can be chosen independently, $A(q,p)$ and $B(q,p)$ must be individually real:

$$\widehat{A} = \widehat{A}^\dagger \quad\Rightarrow\quad A(q,p) = A(q,p)^*. \tag{21}$$

Expression (20) for $A(q,p)$ is indeed the Weyl–Wigner representative of $\widehat{A}$ in phase-space form. With elementary manipulations we can express it in the familiar forms

$$A(q,p) = 2\int\!\!\int \mathrm{d}q'\,\mathrm{d}p'\,A_l(q',p')\exp\{2\mathrm{i}(q-q')(p-p')/\hbar\} \tag{22}$$

$$= \int\!\!\int \mathrm{d}q'\left\langle q-\frac{1}{2}q'\right|\widehat{A}\left|q+\frac{1}{2}q'\right\rangle\exp\{\mathrm{i}pq'/\hbar\} \tag{23}$$

or

$$A(q,p) = 2\pi\hbar\,\mathrm{Tr}\{\widehat{A}\widehat{\mathcal{W}}(q,p)\}, \tag{24}$$

where

$$\begin{aligned}\widehat{\mathcal{W}}(q,p) &= \frac{1}{2\pi\hbar}\int\!\!\int \mathrm{d}q'\left|q+\frac{1}{2}q'\right\rangle\left\langle q-\frac{1}{2}q'\right|\exp\{\mathrm{i}pq'/\hbar\}\\ &= \int\!\!\int \mathrm{d}q'\left|q+\frac{1}{2}q'\right\rangle\left\langle q+\frac{1}{2}q'|p\right\rangle\left\langle p|q-\frac{1}{2}q'\right\rangle\left\langle q-\frac{1}{2}q'\right|.\end{aligned} \tag{25}$$

[9] It is interesting that while as a function of four phase-space variables ξ is the pointwise *square* of K_l, as a kernel it is the *square root* of K_l.

[10] The factor in equation (19) is chosen so that $\widehat{A}$ and $A(q,p)$ have the same physical dimension.

Representing this 'phase-point operator' as[11]

$$\widehat{\mathcal{W}}(q,p) = \int \mathrm{d}q'\,\mathrm{d}q''|q'\rangle\langle q'|\widehat{\mathcal{W}}(q,p)|q''\rangle\langle q''|, \tag{26}$$

the matrix elements are given by

$$\langle q'|\widehat{\mathcal{W}}(q,p)|q''\rangle = \frac{1}{\pi\hbar}\delta(q'+q''-2q)\exp\{\mathrm{i}p(q'-q'')/\hbar\}. \tag{27}$$

It is evident from the first line in equation (25) that $\widehat{\mathcal{W}}(q,p)$ is Hermitian as well as that

$$\mathrm{Tr}\{\widehat{\mathcal{W}}(q,p)\} = \frac{1}{2\pi\hbar}. \tag{28}$$

The Weyl correspondence makes use (see below) of the 'Weyl operators' $\exp\{\mathrm{i}(x\widehat{p} - k\widehat{q})/\hbar\}$ that are labelled by the phase-space points x and k. Then, one can prove that

$$\widehat{\mathcal{W}}(q,p) = \int\int \frac{\mathrm{d}x\,\mathrm{d}k}{(2\pi\hbar)^2}\exp\{-\mathrm{i}(xp-kq)\}\exp\{\mathrm{i}(x\widehat{p}-k\widehat{q})/\hbar\}, \tag{29}$$

i.e. that the phase-point operators are the symplectic Fourier transforms of the Weyl operators. Indeed, a straightforward calculation shows that

$$\langle q'|\exp\{\mathrm{i}(x\widehat{p}-k\widehat{q})/\hbar\}|q''\rangle = \delta(x+q'-q'')\exp\left\{-\mathrm{i}k\frac{q'+q''}{2\hbar}\right\} \tag{30}$$

and using this result to evaluate the matrix elements of both sides of equation (29) one obtains back equation (27).

We summarize this procedure as follows: the introduction of phase-space description of operators is via the Dirac method and is quite elementary; at the next stage we carry out a simple transformation to remove the kernel present in the trace expression, and this leads to the Wigner–Weyl result.

The general Weyl association is that contained in equations (20), (24) and (25). For the density operator $\widehat{\rho}$ we use a different normalization and define the Wigner function by

$$\rho(q,p) = \mathrm{Tr}\{\widehat{\rho}\widehat{\mathcal{W}}(q,p)\} \tag{31}$$

so that the expectation of $\widehat{A}$ in $\widehat{\rho}$ is

$$\mathrm{Tr}\{\widehat{\rho}\widehat{A}\} = \int\int \mathrm{d}q\,\mathrm{d}p\,\rho(q,p)A(q,p). \tag{32}$$

For any $\widehat{A}$, upon integration the Dirac representatives reproduce the marginals as in equations (7), and (9). When these are combined with equation (17) for $\xi(q,p;q',p')$ we at once get

$$\int \mathrm{d}p\,A(q,p) = 2\pi\hbar\langle q|\widehat{A}|q\rangle, \qquad \int \mathrm{d}q\,A(q,p) = 2\pi\hbar\langle p|\widehat{A}|p\rangle. \tag{33}$$

For the density operator $\widehat{\rho}$ we omit the factor $2\pi\hbar$, so the marginal probability distributions are recovered again via a two-step process as

$$\int \mathrm{d}p\,\rho(q,p) = \langle q|\widehat{\rho}|q\rangle, \qquad \int \mathrm{d}q\,\rho(q,p) = \langle p|\widehat{\rho}|p\rangle. \tag{34}$$

[11] The operators $\widehat{W}(q,p)$ have been studied in [27], they have been called the elements of the 'Wigner basis' for the space of operators. In the work of Wootters [6] they have been called 'phase-point operators'.

4. Kinematics of an N-level quantum system

We now take up the question of adapting the Dirac procedure to the finite-dimensional case. We consider a quantum system whose state space is a complex (finite-dimensional) Hilbert space $\mathcal{H}^{(N)}$ of dimension N. We select a particular orthonormal basis for $\mathcal{H}^{(N)}$, written as $|q\rangle$, with $q = 0, 1, \ldots, N-1$, to be called the set of 'position eigenstates' of the system. Then:

$$\langle q|q'\rangle = \delta_{qq'}, \qquad q, q' = 0, 1, \ldots, N-1; \qquad \sum_{q=0}^{N-1} |q\rangle\langle q| = \mathbb{I}. \tag{35}$$

A general vector $|\psi\rangle \in \mathcal{H}^{(N)}$ is described in this basis by a corresponding wavefunction which is an N-component complex column vector:

$$\begin{aligned}&\psi(q) = \langle q|\psi\rangle,\\ &\langle\psi|\psi\rangle = \|\psi\|^2 = \sum_{q=0}^{N-1}\langle\psi|q\rangle\langle q|\psi\rangle = \sum_{q=0}^{N-1}|\psi(q)|^2.\end{aligned} \tag{36}$$

By means of an N-point Fourier series transformation we arrive at a complementary orthonormal basis of 'momentum eigenstates' $|p\rangle$ with $p = 0, 1, \ldots, N-1$. The principal equations are as follows:

$$\begin{aligned}&|p\rangle = \frac{1}{\sqrt{N}}\sum_{q=0}^{N-1} \mathrm{e}^{2\pi\,\mathrm{i}qp/N}|q\rangle, \qquad \langle p|p'\rangle = \delta_{pp'}, \quad p, p' = 0, 1, \ldots, N-1,\\ &\sum_{p=0}^{N-1} |p\rangle\langle p| = \mathbb{I}, \qquad \langle q|p\rangle = \frac{1}{\sqrt{N}}\,\mathrm{e}^{2\pi\,\mathrm{i}qp/N}.\end{aligned} \tag{37}$$

Now consider a general operator $\widehat{A}$ on $\mathcal{H}^{(N)}$. Using either the basis $\{|q\rangle\}$ or the basis $\{|p\rangle\}$ for $\mathcal{H}^{(N)}$, it can be completely described by the corresponding $N \times N$ square complex matrices $\langle q'|\widehat{A}|q\rangle$ or $\langle p'|\widehat{A}|p\rangle$. Following the method of Dirac, however, we can equally well describe $\widehat{A}$ completely by the collection of 'mixed matrix elements' $\langle q|\widehat{A}|p\rangle$; we call this an $N \times N$ 'array' rather than a matrix since operator multiplication is not simply the multiplication of these arrays thought of as matrices. We also note that with the introduction of such arrays the step to a 'phase-space' description of $\widehat{A}$ has been taken. More precisely, we define the (left) phase-space representative of $\widehat{A}$ by

$$A_l(q, p) = \langle q|\widehat{A}|p\rangle\langle p|q\rangle = \mathrm{Tr}\{\widehat{A}|p\rangle\langle p|q\rangle\langle q|\} = \frac{1}{\sqrt{N}}\langle q|\widehat{A}|p\rangle \exp\{-2\pi\mathrm{i}pq/N\}. \tag{38}$$

(By interchanging the roles of q and p we can equally well define an expression $A_r(q, p) = \langle p|\widehat{A}|q\rangle\langle q|p\rangle$; however, we will work with the quantities $A_l(q, p)$.) The following are immediate consequences of this definition:

$$\sum_p A_l(q, p) = \langle q|\widehat{A}|q\rangle, \qquad \sum_q A_l(q, p) = \langle p|\widehat{A}|p\rangle, \qquad \sum_{q,p} A_l(q, p) = \mathrm{Tr}\{\widehat{A}\}. \tag{39}$$

We may note at this point that as in the continuous case, even for Hermitian $\widehat{A}$, $A_l(q, p)$ is in general complex.

Now take two operators $\widehat{A}$ and $\widehat{B}$ and the trace of their product. We express this in terms of their (left) phase-space representatives as follows:

$$\begin{aligned}\mathrm{Tr}\{\widehat{A}\widehat{B}\} &= N\sum_{q,p} A_l(q, p)B_r(q, p) = \sum_{q,p}\sum_{q',p'}\langle q|\widehat{A}|p\rangle\langle p|q'\rangle\langle q'|\widehat{B}|p'\rangle\langle p'|q\rangle\\ &= \sum_{q,p}\sum_{q',p'} A_l(q, p)K_l(q, p; q', p')B_l(q', p'),\end{aligned} \tag{40}$$

where

$$K_l(q, p; q', p') = N^2\langle q|p\rangle\langle p|q'\rangle\langle q'|p'\rangle\langle p'|q\rangle = \exp\{2\pi \mathrm{i}(q-q')(p-p')/N\}. \tag{41}$$

Thus, the matrix phase-space kernel K_l analogous to equation (13) has been introduced. We note in passing that (apart from the N^2 factor) it is a four-vertex Bargmann invariant, so its phase is an instance of the kinematic geometric phase [28].

The study of the detailed properties of K_l will lead us to the solution of setting up a physically reasonable Wigner distribution, *for any value of the dimension N*.

5. Properties of the kernel K_l

We can regard $K_l(q, p; q', p')$ as defined in equation (41) as constituting a complex square matrix of dimension N^2, with the first pair of arguments (q, p) being row index and the second pair (q', p') column index[12]. We denote by $\mathcal{K}^{(N^2)}$ a complex linear space of dimension N^2, made up of vectors f with components $f(q, p)$:

$$f \in \mathcal{K}^{(N^2)} \to f(q, p), \qquad q, p = 0, 1, 2 \ldots, N-1. \tag{42}$$

It is to be understood that these vectors are 'periodic' in the sense that

$$f(q+nN, p+n'N) = f(q, p), \qquad n, n' = 0, \pm 1, \pm 2, \ldots. \tag{43}$$

The norm is defined in the natural way by

$$\|f\|^2 = (f, f) = \sum_{q,p=0,1,\ldots}^{N-1} |f(q, p)|^2. \tag{44}$$

Then K_l acts on such vectors according to

$$(K_l f)(q, p) = \sum_{q',p'} K_l(q, p; q', p') f(q', p'). \tag{45}$$

The following properties are immediately evident

- symmetry:

$$K_l(q, p; q', p') = K_l(q', p'; q, p); \tag{46}$$

- essential unitarity:

$$\sum_{q',p'} K_l(q, p; q', p') K_l(q'', p''; q', p')^* = N^2 \delta_{qq''}\delta_{pp''}; \tag{47}$$

- translation invariance:

$$\begin{aligned} &K_l(q+q_0, p+p_0; q'+q_0, p'+p_0) = K_l(q, p; q', p'),\\ &q_0, p_0 = 0, 1, 2, \ldots, N-1. \end{aligned} \tag{48}$$

Here and in the following we interpret translated arguments $q+q_0$, $p+p_0, \ldots$ as always taken modulo N, so that they always lie in the range $0, 1, \ldots, N-1$. Property (47) means that any eigenvalue of K_l is of the form $N\,\mathrm{e}^{\mathrm{i}\varphi}$ for some phase φ. In addition to the above, the following 'marginals' properties are also evident from definition (41):

$$\sum_{p'} K_l(q, p; q', p') = N\delta_{qq'}, \qquad \text{independent of } p, \tag{49a}$$

[12] We introduce below a more compact efficient notation to express this.

$$\sum_{q'} K_l(q,p;q',p') = N\delta_{pp'}, \qquad \text{independent of } q. \tag{49b}$$

These are particularly important for the Wigner distribution problem, so we explore them in some detail and relate them to the eigenvalue and eigenvector properties of K_l. From either one of equations (49*a*), (49*b*) we get the (weaker) relations

$$\sum_{q'p'} K_l(q,p;q',p') = N, \qquad \text{independent of } q, p. \tag{50}$$

Let us introduce a single symbol σ to denote the pair (q, p) by the definition

$$\sigma = qN + p + 1. \tag{51}$$

Thus σ runs from 1 to N^2. For summations and Kronecker symbols we have the rules

$$\begin{aligned}
&\sum_{\substack{p\\ q \text{ fixed}}} \cdots = \sum_{\sigma = qN+1, qN+2 \ldots (q+1)N} \cdots, \\
&\sum_{\substack{q\\ p \text{ fixed}}} \cdots = \sum_{\sigma = p+1, N+p+1, 2N+p+1, \ldots, (N-1)N+p+1} \cdots, \\
&\sum_{qp} \cdots = \sum_{\sigma=1}^{N^2} \cdots, \\
&\delta_{\sigma\sigma'} = \delta_{qq'}\delta_{pp'}.
\end{aligned} \tag{52}$$

We hereafter use σ or q, p interchangeably as convenient. The kernel $K_l(q, p; q', p')$ can now be written as $K_l(\sigma; \sigma')$, while vectors $f \in \mathcal{K}^{(N^2)}$ have components $f(\sigma)$. In addition to the properties (46), (47), (49*a*), (49*b*) and (50) we have the trace property following from (41):

$$\mathrm{Tr}\{K_l\} = \sum_{\sigma} K_l(\sigma, \sigma) = N^2. \tag{53}$$

With this notation one can now see that the marginals properties (49*a*), (49*b*) can be expressed as follows: for each $q' = 0, 1, \ldots, N-1$ we define a vector $U_{q'}$ in $\mathcal{K}^{(N^2)}$, forming altogether a set of N real orthonormal vectors (not a basis!) by

$$\begin{aligned}
&U_{q'}(\sigma) = \frac{1}{\sqrt{N}}\delta_{qq'}, \qquad \text{independent of } p, \\
&(U_{q'}, U_q) = \delta_{q'\,q}.
\end{aligned} \tag{54}$$

Then equation (49*a*) translates exactly into the statement

$$K_l U_q = N U_q, \qquad q = 0, 1, \ldots, N-1. \tag{55}$$

Similarly, for each $p' = 0, 1, \ldots, N-1$ we define a vector $V_{p'}$ in $\mathcal{K}^{(N^2)}$ forming altogether a set of N real orthonormal vectors (again, not a basis!) by

$$\begin{aligned}
&V_{p'}(\sigma) = \frac{1}{\sqrt{N}}\delta_{pp'}, \qquad \text{independent of } q, \\
&(V_{p'}, V_p) = \delta_{p'p}.
\end{aligned} \tag{56}$$

Then equation (49*b*) translates into

$$K_l V_p = N V_p, \qquad p = 0, 1, \ldots, N-1. \tag{57}$$

These real eigenvectors U_q and V_p are mutually non-orthogonal:

$$(V_p, U_q) = \sum_{\sigma'} V_p(\sigma') U_q(\sigma') = \frac{1}{N}. \tag{58}$$

This leads to the single linear dependence relation among the $2N$ (real) vectors U_q, V_p

$$\sum_q U_q\text{s} = \sum_p V_p\text{s}, \tag{59}$$

which can also be read off from equations (54) and (56). Therefore, U_qs and V_ps together span a $(2N-1)$-dimensional subspace $\mathcal{K}^{(2N-1)}$ in $\mathcal{K}^{(N^2)}$, over which K_l reduces to N times the identity. We can construct an orthonormal basis of $(2N-1)$ real vectors for $\mathcal{K}^{(2N-1)}$ for instance by the following recipe:

$$\begin{aligned}
&\Psi_0 = \frac{1}{\sqrt{N}}\sum_q U_q = \frac{1}{\sqrt{N}}\sum_p V_p,\\
&\widetilde{U}_j = \frac{1}{\sqrt{j(j+1)}}(U_0 + U_1 + \cdots + U_{j-1} - jU_j), \qquad j = 1, 2, \ldots, N-1,\\
&\widetilde{V}_j = \frac{1}{\sqrt{j(j+1)}}(V_0 + V_1 + \cdots + V_{j-1} - jV_j), \qquad j = 1, 2, \ldots, N-1,\\
&(\widetilde{U}_{j'}, \widetilde{U}_j) = (\widetilde{V}_{j'}, \widetilde{V}_j) = \delta_{j'j}, \qquad (\Psi_0, \Psi_0) = 1,\\
&(\widetilde{U}_{j'}, \Psi_0) = (\widetilde{V}_{j'}, \Psi_0) = (\widetilde{U}_{j'}, \widetilde{V}_j) = 0.
\end{aligned} \tag{60}$$

If the orthogonal complement of $\mathcal{K}^{(2N-1)}$ in $\mathcal{K}^{(N^2)}$, of dimension $(N-1)^2$, is written as $\mathcal{K}^{(N-1)^2}$, i.e.

$$\mathcal{K}^{(N^2)} = \mathcal{K}^{(2N-1)} \oplus \mathcal{K}^{(N-1)^2}, \tag{61}$$

then we can supplement the basis (60) for $\mathcal{K}^{(2N-1)}$ by (any) additional real orthonormal vectors to span $\mathcal{K}^{(N-1)^2}$. The essential unitarity of K_l means that it leaves $\mathcal{K}^{(N-1)^2}$ also invariant; the transition from the original (standard) basis of $\mathcal{K}^{(N^2)}$ to the present one can be accomplished by an element of the real orthogonal rotation group $SO(N^2)$, thus preserving the symmetry (46) of K_l. Therefore, the matrix K_l has the following structure in a (real) basis adapted to the decomposition (61):

$$K_l \to \begin{pmatrix} \mathbf{N}\cdot\mathbb{I} & \mathbf{0} \\ \mathbf{0} & \mathbf{A} + \mathrm{i}\mathbf{B} \end{pmatrix}. \tag{62}$$

The unit matrix is of dimension $(2N-1)$, while the two real $(N-1)^2$-dimensional matrices $\mathbf{A}$ and $\mathbf{B}$ obey

$$\begin{aligned}
&\mathbf{A}^T = \mathbf{A}, \qquad \mathbf{B}^T = \mathbf{B}, \qquad \mathbf{AB} = \mathbf{BA},\\
&\mathbf{A}^2 + \mathbf{B}^2 = N^2 \cdot \mathbb{I}_{(N-1)^2\times(N-1)^2},\\
&\mathrm{Tr}\{\mathbf{A}\} = -N(N-1), \qquad \mathrm{Tr}\{\mathbf{B}\} = 0.
\end{aligned} \tag{63}$$

Thus the matrix $\mathbf{A}+\mathrm{i}\mathbf{B}$ can definitely be diagonalized by a real rotation in $(N-1)^2$ dimensions, i.e., by an element of $SO((N-1)^2)$, and each eigenvalue of $\mathbf{A}+\mathrm{i}\mathbf{B}$ is of the form $N\,\mathrm{e}^{\mathrm{i}\varphi}$ for some angle φ.

It now turns out that we can carry through this diagonalization process explicitly. The translation invariance (48) of K_l means that the eigenvectors of K_l can be constructed as 'plane waves' in phase space. We can obtain a complete real orthonormal set of vectors of K_l in $\mathcal{K}^{(N^2)}$ by this route, recovering the subset of eigenvectors (60) as part of a complete set.

For each point $\sigma_0 = (q_0, p_0)$ we define a unit vector χ_{σ_0} with components

$$\chi_{\sigma_0}(\sigma) = \frac{1}{N}\exp(2\pi\mathrm{i}(q_0 p + p_0 q)/N) \tag{64}$$

(we see that condition (43) is indeed obeyed). Thus, we have exactly N^2 vectors χ_{σ_0}. Using the modulo N rule for phase-space arguments we then easily obtain the following:

$$K_l \chi_{\sigma_0} = N\,\mathrm{e}^{-2\pi \mathrm{i} q_0 p_0/N} \chi_{\sigma_0}, \tag{65a}$$

$$\left(\chi_{\sigma_0'}, \chi_{\sigma_0}\right) = \delta_{\sigma_0'\sigma_0}. \tag{65b}$$

Therefore, we have achieved full diagonalization of K_l, with $\{\chi_{\sigma_0}\}$ forming an orthonormal basis in $\mathcal{K}^{(N^2)}$. The previously found (real) basis for the subspace $\mathcal{K}^{(2N-1)}$, made up exclusively of eigenvectors of K_l with eigenvalues N, is essentially the subset of $(2N-1)$ vectors $\chi_{q_0,0}$ for $q_0 = 0, 1, \ldots, N-1$ and χ_{0,p_0} for $p_0 = 1, \ldots, N-1$. Indeed, we find

$$U_q = \frac{1}{\sqrt{N}} \sum_{p_0=0}^{N-1} \mathrm{e}^{-2\pi \mathrm{i} q p_0/N} \chi_{0,p_0}, \qquad V_p = \frac{1}{\sqrt{N}} \sum_{q_0=0}^{N-1} \mathrm{e}^{-2\pi \mathrm{i} q_0 p/N} \chi_{q_0,0}. \tag{66}$$

The remaining $(N-1)^2$ eigenvectors χ_{σ_0} for $q_0, p_0 = 1, 2, \ldots, N-1$ span the orthogonal subspace $\mathcal{K}^{(N-1)^2}$. Here we have in detail the following structure. The two eigenvectors χ_{q_0,p_0} and $\chi_{N-q_0,N-p_0}$ are degenerate, and their components are related by complex conjugation:

$$\begin{aligned} &K_l \chi_{q_0,p_0} = N\,\mathrm{e}^{-2\pi \mathrm{i} q_0 p_0/N} \chi_{q_0,p_0}, \\ &K_l \chi_{N-q_0,N-p_0} = N\,\mathrm{e}^{-2\pi \mathrm{i} q_0 p_0/N} \chi_{N-q_0,N-p_0}; \\ &\chi_{N-q_0,N-p_0}(\sigma) = \chi_{q_0,p_0}(\sigma)^*. \end{aligned} \tag{67}$$

Therefore, we have a pattern that depends on the parity of N. For odd N, we have $(N-1)^2/2$ distinct degenerate pairs of mutually complex conjugate orthogonal eigenvectors $\{\chi_{q_0,p_0}, \chi_{N-q_0,N-p_0}\}$ for $q_0 = 1, 2, \ldots, (N-1)/2$ and $p_0 = 1, 2, \ldots, N-1$. For even N we have one real eigenvector $\chi_{N/2,N/2}$ with eigenvalue $N(-1)^{N/2}$ followed by $((N-1)^2-1)/2$ distinct degenerate pairs $\{\chi_{q_0,p_0}, \chi_{N-q_0,N-p_0}\}$ where we omit $q_0 = p_0 = N/2$. In either case it is clear that by passing to the real and imaginary parts of χ_{q_0,p_0}, while leaving $\chi_{N/2,N/2}$ unchanged, we get a real orthonormal basis for $\mathcal{K}^{(N-1)^2}$ in which the matrix $\mathbf{A} + \mathrm{i}\mathbf{B}$ of equation (62) is diagonal.

Equipped with these important properties of K_l we turn to equation (40) from where we can find the route to the Wigner distribution.

6. The kernel ξ and the Wigner distribution

Motivated by the structure (40) for $\mathrm{Tr}\{\widehat{A}\widehat{B}\}$ for two general operators $\widehat{A}$ and $\widehat{B}$ on $\mathcal{H}^{(N)}$, we try to express the kernel $K_l(q, p; q', p')$ in the form

$$K_l(\sigma, \sigma') = \sum_{\sigma''} \xi(\sigma'', \sigma)\xi(\sigma'', \sigma'), \tag{68}$$

with suitable conditions imposed on ξ. The desirable conditions are, as with K_l itself: symmetry, essential unitarity, translation invariance and marginal conditions similar to equations (49*b*) and (49*b*) for K_l:

$$\xi(\sigma, \sigma') = \xi(\sigma', \sigma), \tag{69a}$$

$$\sum_{\sigma'} \xi(\sigma, \sigma')\xi(\sigma'', \sigma')^* = N\delta_{\sigma\sigma''}, \tag{69b}$$

$$\xi(q + q_0, p + p_0; q' + q_0, p' + p_0) = \xi(q, p; q', p'), \tag{69c}$$

$$\xi U_q = \sqrt{N} U_q, \xi V_p = \sqrt{N} V_p. \tag{69d}$$

Here we have expressed the last marginals conditions already in terms of the eigenvectors (not all independent!) U_q, V_p of K_l lying in $\mathcal{K}^{(2N-1)}$. More explicitly they read

$$\sum_{p'} \xi(q,p;q',p') = \sqrt{N}\delta_{qq'}, \qquad \sum_{q'} \xi(q,p;q',p') = \sqrt{N}\delta_{pp'}. \tag{70}$$

The detailed analysis of the eigenvectors and eigenvalues of K_l in the previous section immediately leads to solutions for ξ. The translation invariance of (69*c*) is ensured by arranging that the 'plane waves' eigenvectors χ_{q_0,p_0} of K_l are eigenvectors of ξ as well. We take ξ to obey

$$\xi\chi_{q_0,0} = \sqrt{N}\chi_{q_0,0}, \qquad q_0 = 0,1,\ldots,N-1; \tag{71a}$$

$$\xi\chi_{0,p_0} = \sqrt{N}\chi_{0,p_0}, \qquad p_0 = 0,1,\ldots,N-1; \tag{71b}$$

$$\begin{aligned}\xi\left(\chi_{q_0,p_0} \text{ or } \chi_{N-q_0,N-p_0}\right) &= \pm\sqrt{N}\,\mathrm{e}^{-\mathrm{i}\pi q_0p_0/N}\left(\chi_{q_0,p_0}\text{or}\chi_{N-q_0,N-p_0}\right),\\ &q_0, p_0 = 1,\ldots,N-1.\end{aligned} \tag{71c}$$

In the subspaces $\mathcal{K}^{(2N-1)}$ and $\mathcal{K}^{(N-1)^2}$ we then have:

$$\begin{aligned}\xi &= \sqrt{N}\cdot\mathbb{I} \quad \text{on} \quad \mathcal{K}^{(2N-1)},\\ \xi &= (\mathbf{A}+\mathrm{i}\mathbf{B})^{1/2} \quad \text{on} \quad \mathcal{K}^{(N-1)^2}.\end{aligned} \tag{72}$$

Equations (71*a*) and (71*b*) ensure the validity of the marginals properties equation (69*d*) or (70) while equation (69*b*) is obeyed by construction. It is the symmetry requirement (69*a*) that dictates that in the case of degenerate orthonormal pairs of K_l eigenvectors $\left\{\chi_{q_0,p_0}, \chi_{N-q_0,N-p_0}\right\}$ we choose the square root of the eigenvalue $N\,\mathrm{e}^{-2\pi\,\mathrm{i}q_0p_0/N}$ of K_l in the same way; this is expressed in equation (71*c*). Thus we see, for odd N there is a $2^{(N-1)^2/2}$-fold freedom in the choice of ξ; for N even there is a $2^{((N-1)^2+1)/2}$-fold freedom. In each case, a particular square root of $\mathbf{A}+\mathrm{i}\mathbf{B}$ is involved in equation (72).

With any such ξ, we can return to equation (40) and write it in a manifestly kernel-independent manner

$$\mathrm{Tr}\{\widehat{A}\widehat{B}\} = N\sum_{q,p} A(q,p)B(q,p), \tag{73}$$

where

$$\begin{aligned}A(q,p) &= \frac{1}{\sqrt{N}}\sum_{q',p'}\xi(q,p;q',p')A_l(q',p')\\ &= \frac{1}{\sqrt{N}}\sum_{q',p'}\xi(q,p;q',p')\langle q'|\widehat{A}|p'\rangle\langle p'|q'\rangle,\end{aligned} \tag{74}$$

with a similar expression for $B(q,p)$ in terms of $\widehat{B}$. We will show below that for Hermitian $\widehat{A}$, $A(q,p)$ is real. Combining equations (39) and (69*d*) we have ensured the marginals properties

$$\sum_p A(q,p) = \langle q|\widehat{A}|q\rangle, \qquad \sum_q A(q,p) = \langle p|\widehat{A}|p\rangle. \tag{75}$$

For the density matrix $\widehat{\rho}$ describing some pure or mixed state of the N-level system, we then have the real Wigner distribution

$$W(q,p) = \frac{1}{\sqrt{N}}\sum_{q',p'}\xi(q,p;q',p')\langle q'|\widehat{\rho}|p'\rangle\langle p'|q'\rangle \tag{76}$$

and by equations (75) the two marginal probability distributions in q and p are immediately recovered. In particular, we find that for position eigenstates and momentum eigenstates the freedom in the choice of ξ (which in any case is limited to its action on $\mathcal{K}^{(N-1)^2}$) does not matter and we get the anticipated results:

$$\begin{aligned} \widehat{\rho} &= |q'\rangle\langle q'| \quad \Rightarrow \quad W(q,p) = \frac{1}{N}\delta_{qq'}, \qquad \text{independent of } p, \\ \widehat{\rho} &= |p'\rangle\langle p'| \quad \Rightarrow \quad W(q,p) = \frac{1}{N}\delta_{pp'}, \qquad \text{independent of } q. \end{aligned} \tag{77}$$

Returning to the Wigner distribution (76) we may rewrite it as

$$W(q,p) = \frac{1}{N}\operatorname{Tr}\{\rho \widehat{W}(q,p)\} \tag{78}$$

by introducing elements of Wigner basis or phase-point operators (see footnote 11)

$$\widehat{W}(q,p) = \sqrt{N}\sum_{q',p'} \xi(q,p;q',p')\langle p'|q'\rangle|p'\rangle\langle q'|. \tag{79}$$

It is an interesting exercise to verify, by combining definition (41) of K_l and (68) and (69b), that these are Hermitian:

$$\widehat{W}(q,p)^\dagger = \widehat{W}(q,p). \tag{80}$$

This proves that $W(q,p)$ and, more generally, $A(q,p) = \operatorname{Tr}\{\widehat{A}\widehat{W}(q,p)\}$ for Hermitian $\widehat{A}$, are both real. In addition one can check, by virtue of equations (68), (69a)–(69d), that they satisfy

$$\operatorname{Tr}\{\widehat{W}(\sigma)\} = 1, \qquad \operatorname{Tr}\{\widehat{W}(\sigma)\widehat{W}(\sigma')\} = N\delta_{\sigma\sigma'}. \tag{81}$$

7. The case of $N = 2$: the qubit

This case is particularly interesting in that some earlier treatments have had to treat it on its own, as distinct from N an odd prime or an odd integer. In the standard basis for the two-dimensional Hilbert space $\mathcal{H}^{(2)}$ made up of $|q\rangle$ for $q = 0, 1$, accompanied by its complementary basis $|p\rangle$, the matrix $K_l(q,p;q',p')$ is the following:

$$K_l = \begin{pmatrix} 1 & 1 & 1 & -1 \\ 1 & 1 & -1 & 1 \\ 1 & -1 & 1 & 1 \\ -1 & 1 & 1 & 1 \end{pmatrix}. \tag{82}$$

The rows and columns are labelled in the sequence: $(q,p) = (0,0), (0,1), (1,0), (1,1)$, and the matrix elements are read off from equation (41). The three orthonormal eigenvectors of K_l with eigenvalue 2, spanning the subspace $\mathcal{K}^{(3)}$ of the general treatment in section 5, are as follows:

$$\Psi_0 = \frac{1}{2}\begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}, \qquad \widetilde{U}_1 = \frac{1}{2}\begin{pmatrix} 1 \\ 1 \\ -1 \\ -1 \end{pmatrix}, \qquad \widetilde{V}_1 = \frac{1}{2}\begin{pmatrix} 1 \\ -1 \\ 1 \\ -1 \end{pmatrix}. \tag{83}$$

We choose the fourth eigenvector of K_l, with eigenvalue necessarily -2 since $\mathrm{Tr}\{K_l\} = 4$, to be

$$W = \frac{1}{2}\begin{pmatrix} 1 \\ -1 \\ -1 \\ 1 \end{pmatrix}. \tag{84}$$

Then the kernel ξ can be immediately synthesized from

$$\xi\Psi_0 = \sqrt{2}\Psi_0, \qquad \xi\widetilde{U}_1 = \sqrt{2}\widetilde{U}_1, \qquad \xi\widetilde{V}_1 = \sqrt{2}\widetilde{V}_1, \qquad \xi W = \mathrm{i}\sqrt{2}W \tag{85}$$

and in the standard basis turns out to be

$$\xi = \frac{1}{2\sqrt{2}}\begin{pmatrix} 3+\mathrm{i} & 1-\mathrm{i} & 1-\mathrm{i} & -1+\mathrm{i} \\ 1-\mathrm{i} & 3+\mathrm{i} & -1+\mathrm{i} & 1-\mathrm{i} \\ 1-\mathrm{i} & -1+\mathrm{i} & 3+\mathrm{i} & 1-\mathrm{i} \\ -1+\mathrm{i} & 1-\mathrm{i} & 1-\mathrm{i} & 3+\mathrm{i} \end{pmatrix}. \tag{86}$$

Using the above matrix elements of ξ in (79) we obtain, for the phase-point operators

$$\begin{aligned} \widehat{\mathcal{W}}(0,0) &= \begin{pmatrix} 1 & \frac{1-\mathrm{i}}{2} \\ \frac{1+\mathrm{i}}{2} & 0 \end{pmatrix}, \qquad & \widehat{\mathcal{W}}(0,1) &= \begin{pmatrix} 0 & \frac{1+\mathrm{i}}{2} \\ \frac{1-\mathrm{i}}{2} & 1 \end{pmatrix}, \\ \widehat{\mathcal{W}}(1,0) &= \begin{pmatrix} 1 & \frac{-1+\mathrm{i}}{2} \\ \frac{-1-\mathrm{i}}{2} & 0 \end{pmatrix}, \qquad & \widehat{\mathcal{W}}(1,1) &= \begin{pmatrix} 0 & \frac{-1-\mathrm{i}}{2} \\ \frac{-1+\mathrm{i}}{2} & 1 \end{pmatrix}, \end{aligned} \tag{87}$$

and thereby recover the results of Feynman [5] and Wootters [6] and hence also the connection between sums of phase-point operators along striations of the qubit phase space [21] and the mutually unbiased bases for $N = 2$.

For the density operator $\widehat{\rho} = \frac{1}{2}(\mathbb{I}_2 + \mathbf{a}\cdot\sigma)$, $\mathbf{a}\cdot\mathbf{a} \leqslant 1$ describing a general state of a qubit one can easily calculate the corresponding Wigner distribution using (76) or (78). The results arranged in the form of a matrix read

$$\begin{pmatrix} 1 + a_1 + a_2 + a_3 & 1 + a_1 - a_2 - a_3 \\ 1 - a_1 - a_2 + a_3 & 1 - a_1 + a_2 - a_3 \end{pmatrix}. \tag{88}$$

Using this result it is instructive to verify the validity of (73) for $\widehat{A} = \widehat{\rho}_1 = \frac{1}{2}(\mathbb{I}_2 + \mathbf{a}\cdot\sigma)$, and $\widehat{B} = \widehat{\rho}_2 = \frac{1}{2}(\mathbb{I}_2 + \mathbf{b}\cdot\sigma)$. Further, it is easily seen from (88) that the maximum positive and maximum negative values of the Wigner distribution for a qubit occur when $|a_1| = |a_2| = |a_3| = 1/\sqrt{3}$.

As a final remark, we note that in calculating the kernel ξ, square root of K_l, we might have chosen W in equation (85) to be the eigenvector corresponding to the eigenvalue $-\mathrm{i}\sqrt{2}$ instead of $+\mathrm{i}\sqrt{2}$. This results in changing +i(−i) with −i(+i) in equations (86) and (87) and thus in an interchange of the role of $\widehat{\mathcal{W}}(0,0)$ and $\widehat{\mathcal{W}}(0,1)$ with $\widehat{\mathcal{W}}(1,0)$ and $\widehat{\mathcal{W}}(1,1)$ respectively. Correspondingly, the coefficient a_2 in equation (88) would change sign everywhere. This, however, can be of no physical consequence as is reflected in the fact that the marginals obtained by summing over q or p are independent of a_2.

8. Concluding remarks

We have shown that by an elementary two-step procedure, which works uniformly for continuous as well as finite-dimensional quantum systems, we can arrive at the Wigner–Weyl description of operators in quantum mechanics. The starting point is Dirac's method of expressing a general quantum dynamical variable as an ordered function of non-commuting position and momentum in the continuous case, and its analogue in the discrete case, with (say) position to the left of momentum. This leads to an expression for the trace of the product of two operators involving a kernel. In both cases, this kernel is found to be intimately related to the well-known Bargmann invariants and hence to the geometric phases of quantum mechanics. At the next step we extract a suitable square root of this kernel, essentially unique in the continuous case and with well characterized sign freedoms in the discrete case, which then yields the Wigner–Weyl correspondence and the associated phase-point operators.

A comprehensive method of handling the finite-dimensional case, based on the more familiar continuous case and using a process of 'descent' or 'quotienting' with respect to a discrete Abelian group of phase-space translations, has been developed by Hannay and Berry [4] (hereafter H–B). We compare our approach with theirs in the following terms. In H–B the starting point is to limit oneself to (ideal, non-normalizable) one-dimensional wavefunctions such that in both position and momentum descriptions one has a sum of equally spaced 'spikes' or delta functions. Consistent with this, one imposes phase-space translational periodicities under translation by suitable integral multiples of the basic lattice spacings Δq, Δp. Thus, one considers position and momentum space wavefunctions:

$$\begin{aligned}
\psi(q) &= \psi(q+\Delta q) = \sum_{n=-\infty}^{\infty} C_n\, \mathrm{e}^{2\pi \mathrm{i} nq/\Delta q};\\
\varphi(p) &= \frac{1}{\sqrt{h}}\int_{-\infty}^{\infty} \mathrm{d}q\, \mathrm{e}^{-\mathrm{i}pq/\hbar}\psi(q) \qquad (89)\\
&= \sqrt{\hbar}\sum_{n=-\infty}^{\infty} C_n \delta(p - nh/\Delta q).
\end{aligned}$$

By imposing an N-step periodicity on the discrete coefficients

$$C_{n+N} = C_n, \qquad (90)$$

and writing the integer n as

$$n = mN + j, \qquad m = 0, \pm 1, \pm 2, \ldots, \qquad j = 0, 1, \ldots, N-1 \qquad (91)$$

these wavefunctions become (using the Poisson summation formula)

$$\begin{aligned}
\psi(q) &= \frac{\Delta q}{N}\sum_{m=-\infty}^{\infty} \tilde{C}_m \delta(q - m\Delta q/N),\\
\tilde{C}_m &= \tilde{C}_{m+N} = \sum_{j=0}^{N-1} C_j\, \mathrm{e}^{2\pi\,\mathrm{i} jm/N}; \qquad (92)\\
\varphi(p) &= \sqrt{\hbar}\sum_{n=-\infty}^{\infty} C_n \delta(p - nh/\Delta q).
\end{aligned}$$

The delta function spacing and the period are $\Delta q/N$, Δq for $\psi(q)$ and $h/\Delta q = \Delta p/N$, Δp, for $\varphi(p)$ where $\Delta q \Delta p = hN$. The passage from the set $\{C_j\}$ to the set $\{\tilde{C}_j\}$ is an N-point finite Fourier transform, appropriate for a finite N-state quantum system. In this approach to the discrete case, the continuum definition of the Wigner distribution leads upon use of equation (92) to the expressions

$$W(q, p) = \frac{1}{h}\int_{-\infty}^{\infty} \mathrm{d}q'\, \psi(q - q'/2)\psi(q + q'/2)^*\, \mathrm{e}^{\mathrm{i}pq'/\hbar}$$

$$= \frac{1}{h}\int_{-\infty}^{\infty} \mathrm{d}p'\varphi(p - p'/2)\varphi(p + p'/2)^* \,\mathrm{e}^{-\mathrm{i}qp'/\hbar}$$

$$= \frac{1}{h}\left(\frac{\Delta q}{N}\right)^2 \sum_{m,m'=-\infty}^{\infty} \tilde{C}_m \tilde{C}^*_{m'} \delta\left(q - \frac{m+m'}{2}\cdot\frac{\Delta q}{N}\right) \mathrm{e}^{\mathrm{i}p(m'-m)\Delta q/N\hbar}$$

$$= \sum_{n,n'=-\infty}^{\infty} C_n C^*_{n'} \delta\left(p - \frac{n+n'}{2}\cdot\frac{\Delta p}{N}\right) \mathrm{e}^{\mathrm{i}q(n-n')\Delta p/N\hbar}. \qquad (93)$$

(The periodicities of C_n, $\tilde{C}_m$ and the Poisson summation formula ensure the consistency of these expressions.) As one may have expected, this distribution has support or ‘spikes’ also at *midpoints* of the original lattice of phase-space points $(m\Delta q/N, n\Delta p/N)$ with accompanying phases. Thus in the H–B method of arriving at the Wigner distribution for N-state quantum systems we find that $W(q, p)$ has support at $4N^2$ discrete phase-space points, though the values at sets of four points are phase related.

In our (and some other) direct approach to the finite-dimensional case, in contrast, it is clear from the outset that the domain of definition of Wigner–Weyl representatives is exactly the ‘classical’ discrete phase-space lattice of just N^2 points (q, p) with $0 \leqslant q, p \leqslant N - 1$. Thus, the midway points seen in equation (93) do not appear. On the other hand our definition, equation (74), of the Wigner–Weyl descriptor $A(q, p)$ of $\widehat{A}$ is such that traciality holds, so $A(q, p)$ does describe $\widehat{A}$ completely.

We comment next on the sign freedom remaining in our definition of the N-state Wigner distribution, residing in the freedom of choice of square root of the matrix $\mathbf{A} + \mathrm{i}\mathbf{B}$ in equation (62). (We emphasize that this freedom is present only in the subspace $\mathcal{K}^{(N-1)^2}$ of $\mathcal{K}^{(N^2)}$, since the orthogonal subspace $\mathcal{K}^{(2N-1)}$ is tied to the recovery of the standard q and p marginal distributions.) It is reasonable to anticipate that this may get resolved by the following considerations: extension of the requirement of recovery of marginals with respect to general foliations of the discrete phase space; behaviour of the terms in the Moyal or star product of two Wigner–Weyl symbols corresponding to non-commutative operator multiplication in an $\hbar$ expansion. In the H–B approach, the continuum Wigner–Weyl description of an operator $\widehat{A}$ is carried along through the quotienting procedure, so the analysis may be expected to be somewhat easier than in the direct treatment of the discrete case.

Comparison of our uniform treatment with Wootter’s method where $N =$ power of 2 and $N =$ odd prime power are handled separately, emphasizes that there is considerable flexibility in setting up the Wigner–Weyl correspondence in the finite-dimensional cases. As has been shown elsewhere [29], at least in the odd N case, there are as many choices as ways of regarding an N-element set as a finite group, at the very least.

In conclusion, the Dirac-inspired approach provides a fresh perspective on questions of quantum tomography in finite state systems, and finite geometries relevant to the quantum information theory. We hope to return to these questions, and those mentioned earlier, elsewhere.

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